

Yang-Lee Zeros of the Triangular Ising Antiferromagnets

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Abstract

Using both the exact enumeration method (microcanonical transfer matrix) for a small system ($L = 9$) and the Wang-Landau Monte Carlo algorithm for large systems to $L = 30$, we obtain the exact and approximate densities of states $g(M, E)$, as a function of magnetization M and exchange energy E , for the triangular-lattice Ising model. Based on the density of states $g(M, E)$, we investigate the phase transition properties of Yang-Lee zeros for the triangular Ising antiferromagnets and obtain the magnetic exponents at various temperatures.

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In 1952, it was proposed by Yang and Lee a new theory for explaining the occurrence of phase transitions in the thermodynamic limit [1, 2]. They reinterpreted the partition function as a polynomial of the exponential variable including magnetic field βH . They proposed that in the thermodynamic limit the real axis cross of the complex zero set of the polynomial is directly related to the phase transition. They illustrated their approach by solving the lattice gas (ferromagnetic Ising model in a magnetic field) problem exactly. Later on, along with computational developments this approach has been extended to treating other exponential variables like the exponential term including temperature by Fisher and others [3]. In various applications, computational improvements enabled researchers to get the exact or approximate density of states (DOS) of the finite systems [4, 5, 6, 7, 8, 9, 10, 11, 12, 13]. However, the extraction of the density of zeros for a finite and numerically accessible lattice sizes had been considered very challenging. In recent years, there have been some attempts to overcome the difficulties [14].

Exact DOS can be obtained only for very finite systems like up to the linear size $L = 9$ for the bipartite system on the two dimensional (2D) triangular lattice with nearest neighbour interactions [15, 16]. However, approximate methods like the Wang-Landau sampling [4, 6, 7, 8] can obtain DOS of the quite large finite systems, for example, up to $L = 30$ for the bipartite system on the 2D triangular lattices with nearest neighbour interactions [15].

In this paper, as a series of investigation for the 2D triangular lattice systems with nearest neighbour interactions [15, 16, 17] Yang-Lee zeros are investigated. We construct a high-degree polynomial to get Yang-Lee zero set using the density of states from [15]. In this case, the Hamiltonian \mathcal{H} is given as follows;

$$\mathcal{H} = -J \sum_{i,j} \sigma_i \sigma_j - H \sum_i \sigma_i, \quad (1)$$

where $E = \sum_{\langle i,j \rangle} \sigma_i \sigma_j$ is the exchange energy, $M = \sum_{i=1}^N \sigma_i$ the total magnetization, J the coupling constant ($J > 0$ for ferromagnets (FM) and $J < 0$ for antiferromagnets (AFM): In this paper, for simplicity we take $J = -1$), $\langle i, j \rangle$ denotes distinct pairs of nearest neighbor sites, H the external magnetic field and $\sigma_i = \pm 1$. The polynomial is

$$Z(a, x) = \sum_E \left[\sum_M g(M, E) a^E \right] x^M. \quad (2)$$

Here, $a = e^{-2\beta}$, $x = e^{-2h}$ and the reduced magnetic field $h = \beta H$.

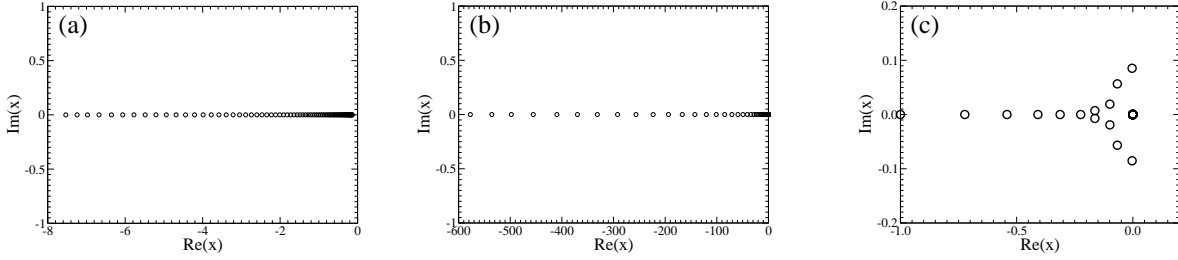


FIG. 1: Yang-Lee zeros in the complex x plane of the 9×9 triangular AF Ising model with periodic boundary conditions: (a) $a = 0.9$, (b) $a = 0.5$, and (c) $a = 0.2$.

At first, using the exact density of states (for $L = 9$) we investigate the Yang-Lee zeros in the complex x plane at several different temperatures, $a = 0.2$, 0.5 and 0.9 . Figure 1 shows the Yang-Lee Zeros in the complex x plane of the 9×9 AF Ising model with the periodic boundary conditions. At high temperatures like $a = 0.9$ and 0.5 , all zeros lie in the left half plane (Fig. 1 (a) and (b)). As the temperature decreases, some of them move toward the right half plane. At low enough temperatures like Fig. 1 (c), where there are phase transitions (see Fig. 2), the Yang-Lee zeros begin to appear in the right half plane.

It is well known the phase diagram of the triangular antiferromagnets in temperature-magnetic field plane [17, 18, 19, 20, 21]. In the phase diagram, it is noted that there are two critical magnetic fields for a given critical temperature because of the critical line shape of the phase diagram. Figure 2 shows the typical phase diagram in reduced temperature-magnetic field plane. We use the terms, “low” ($x > 0.012$) and “high” ($x < 0.012$) reduced magnetic fields.

For several temperatures, $a = 0.05$, 0.1 , 0.15 and 0.2 , we obtain the Yang-Lee zeros for different system sizes (three multiples from 9 to 30) and investigate whether there is the real axis cross of the first Yang-Lee zeros in the thermodynamic limit. In an illustrated Fig. 3, we show the first Yang-Lee zeros for the various system sizes in high (3 (a)) and low (3 (b)) magnetic fields at $a = 0.2$. In the figure, it should be observed that the two graphs (a) and (b) are in completely different scales. For a given temperature a , the Yang-Lee zeros for low and high magnetic fields are in completely different scales in one Yang-Lee zero solution plane. As a typical example in Fig. 4, the Yang-Lee zeros are shown in high and low magnetic fields.

Table I illustrates the real and imaginary parts of the first zeros x_1 at $a = 0.2$ in the high

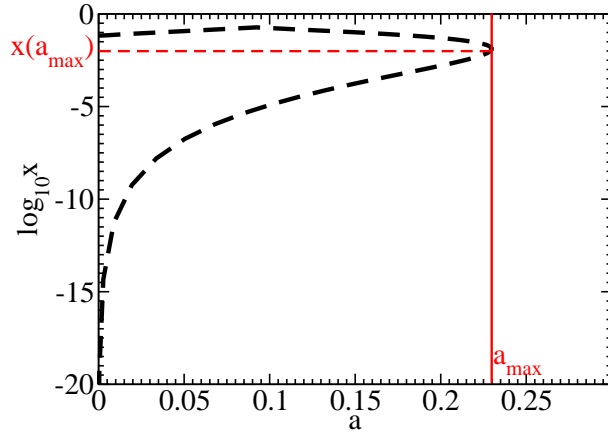


FIG. 2: Typical phase diagram (black dotted line) of the triangular AF Ising model [17]. Below $a_{max} \approx 0.23$ (red solid line), for a given critical temperature a there are two critical magnetic fields. The critical value of $x(a_{max})$, corresponding to $a_{max} \approx 0.23$, is approximately 0.012.

magnetic field for $L = 9-30$ (three multiples). Using the Bulirsch-Stoer algorithm [5, 22], we extrapolated our results for the finite lattices to infinite size and obtained $x_1 = 0.0019(5) - 0.00001(9)i$, indicating the phase transition of the AF Ising model in an external magnetic field. Note that we use approximate density of states from Monte Carlo results for large systems ($L = 12 - 30$, three multiples) so that there are some errors even in the first Yang-Lee zeros. For example, in our data (second column in Table II), the imaginary part of the first zero at infinite size for $a = 0.05$ (low) is positive with much error, we believe, due to the well-known strong crossover effects [23] for low magnetic fields. In thermodynamic limit, if there is a phase transition, the imaginary part of the first zero should be zero if we use exact first zeros for the extrapolation to infinite size and the extrapolation is exact. However, it should be also mentioned that overall the first zeros of approximate density of states from Monte Carlo results are very reliable (for example, in the triangular lattices for $L = 9$, the first zeros of exact density of states at the first line in Table I are exactly the same to the first zeros of approximate density of states from Monte Carlo results).

Also, we can obtain the magnetic scaling exponent for the finite linear size L [24]

$$y_h(L) = -\frac{\ln\{\text{Im}[x_1(L+3)]/\text{Im}[x_1(L)]\}}{\ln[(L+3)/L]}, \quad (3)$$

where x_1 is the first zero. The fourth column of Table I shows the values of the scaling

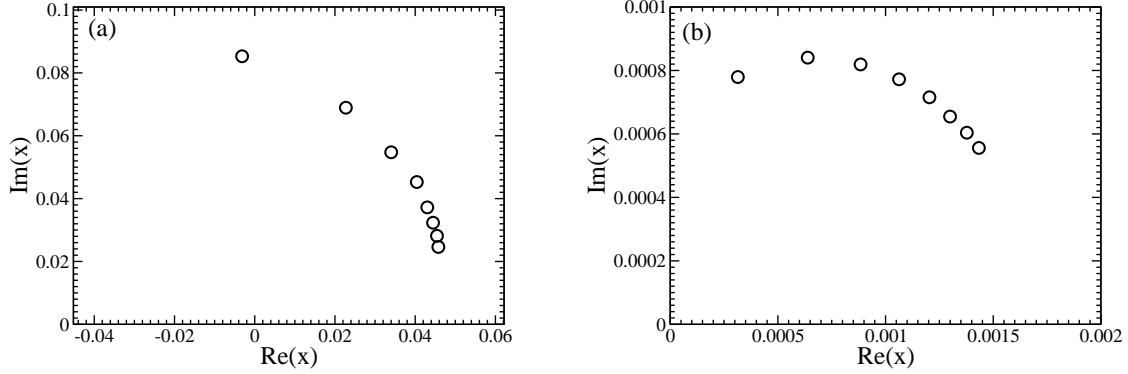


FIG. 3: First Yang-Lee zeros of the various system sizes, $L = 9 - 30$ (three multiples) (a) in low and (b) high magnetic fields at $a = 0.2$:

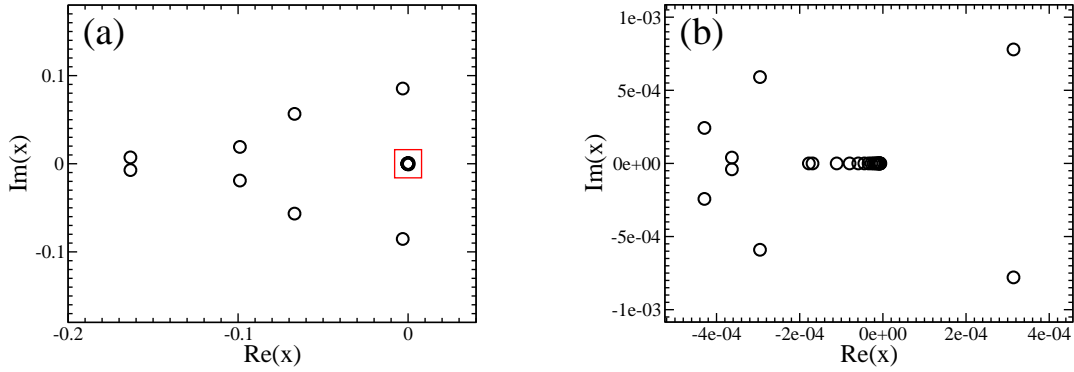


FIG. 4: Figures of Yang-Lee zeros in the complex x plane of the 9×9 triangular AF Ising model with periodic boundary conditions at $a = 0.2$: (a) in low magnetic field ($\text{Re}(x) \sim 0.01$), and (b) in high magnetic field ($\text{Re}(x) \ll 0.01$), zoomed-in figure around the origin of the left figure (boxed area).

magnetic exponent $y_h(L)$. The extrapolated value is $y_h = 1.30$ at $a = 0.2$ in the high magnetic field. Similarly, in the thermodynamic limit we have obtained x_c and y_h for $a = 0.05, 0.1, 0.15$ and 0.2 . They are tabulated in Table II. The evaluated y_h ranges from 1.3 to 1.7 depending on the temperature a [25]. It is known that for $h = 6$ and $T = 0$ the triangular antiferromagnets map onto Baxter's hard-hexagon lattice gas of which the critical exponents are exactly known [20, 26]. In Table II, we observe that as the value a decreases in high magnetic fields y_h gets bigger to $28/15$. The estimated y_h values may

TABLE I: Real and imaginary parts of the first zeros x_1 at $a = 0.2$ for $L = 9 - 30$ (three multiples) in the high magnetic field. $y_h(L)$ is the scaling exponent calculated by Eq. 3. The last row is the extrapolation to infinite size.

L	$\text{Re}(x_1)$	$\text{Im}(x_1)$	$y_h(L)$
9	0.0003141075	0.0007793222	-0.262
12	0.0006385131	0.0008404157	0.115
15	0.0008840487	0.0008190623	0.323
18	0.0010628038	0.0007721926	0.495
21	0.0012038568	0.0007154301	0.663
24	0.0012996089	0.0006547772	0.687
27	0.0013774157	0.0006038531	0.787
30	0.0014334636	0.0005557930	
∞	0.0019(5)	-0.00001(9)	1.297(28)

indicate that the triangular Ising antiferromagnets belong to the three-state Potts class for high magnetic fields but not to the class for intermediate (around $h = 3$) and low magnetic fields. These results contradict with the previous results [21, 25], which say that the phase transition belongs to the 3-state Potts universality class over the whole phase boundary (that means that y_h should be $28/15$ in the whole phase boundary). This might say that our results reflect the well-known strong crossover effects [23] for intermediate (around $h = 3$) and low magnetic fields and slow convergence of y_h . More research is required on this matter.

As a whole, from the imaginary parts of the second column in Table II, it is confirmed that there are phase transitions in external magnetic fields for the various temperatures.

TABLE II: The critical points $x_c(a)$ and the magnetic scaling exponent y_h vs a , in the limit $L \rightarrow \infty$: “low” and “high” represent low and high magnetic fields respectively for the same a . Note that there is no phase transition for high temperatures, that is, large a values (see Fig. 2).

a	x_c	y_h
0.05 (low)	$0.8(2) + 0.17(3)i$	1.7(1)
0.1 (low)	$0.22(6) + 0.02(4)i$	1.7(3)
0.15 (low)	$0.102(7) + 0.1(1)i$	1.61(8)
0.2 (low)	$0.046(4) - 0.4(4)i$	1.5(1)
0.05 (high)	$1.83(3)e-7 + 0.0(1)e-7i$	1.44(1)
0.1 (high)	$1.31(5)e-5 - 0.97(16)e-6i$	1.38(4)
0.15 (high)	$1.9(1)e-4 - 0.0(4)e-4i$	1.49(2)
0.2 (high)	$1.9(5)e-3 - 0.1(9)e-4i$	1.297(28)

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